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Modelling of dissolved oxygen (DO) in a reservoir using artificial neural networks: Amir Kabir Reservoir, Iran

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Abstract. We applied multilayer perceptron (MLP) and radial basis function (RBF) neural network in upstream and downstream water quality stations of the Karaj Reservoir in Iran. For both neural networks, inputs were pH, turbidity, temperature, chlorophyll-a, biochemical oxygen demand (BOD) and nitrate, and the output was dissolved oxygen (DO). We used an MLP neural network with two hidden layers, for upstream station 15 and 33 neurons in the first and second layers respectively, and for the downstream station, 16 and 21 neurons in the first and second hidden layer were used which had minimum amount of errors. For learning process 6-fold cross validation were applied to avoid over fitting. The best results acquired from RBF model, in which the mean bias error (MBE) and root mean squared error (RMSE) were 0.063 and 0.10 for the upstream station. The MBE and RSME were 0.0126 and 0.099 for the downstream station. The coefficient of determination (R^2) between the observed data and the predicted data for upstream and downstream stations in the MLP was 0.801 and 0.904, respectively, and in the RBF network were 0.962 and 0.97, respectively. The MLP neural network had acceptable results; however, the results of RBF network were more accurate. A sensitivity analysis for the MLP neural network indicated that temperature was the first parameter, pH the second and nitrate was the last factor affecting the prediction of DO concentrations. The results proved the workability and accuracy of the RBF model in the prediction of the DO.

Keywords: water quality prediction; the MLP neural network; the RBF neural network; dissolved oxygen; Amir Kabir Reservoir

1. Introduction

Dissolved Oxygen (DO) is a significant water quality parameter for aquatic life and other uses of water. The DO level is a measure of the health of aquatic systems and a certain level of it is essential for the survival of aquatic life. The amount of dissolved oxygen is an important indicator of water quality especially in reservoirs. Generally, in water quality management, analyzing different physical, chemical and biological parameters of rivers and reservoirs need numerous computational approaches.

Oxygen demand can be a result of respiration of algae in a sample and possible oxidation of ammonia. Presence of toxic substances in samples may also affect microbial activity and cause

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changes in DO concentrations (Chen *et al*. 2014). Water quality factors such as DO, generally need to be specified simultaneously. Therefore, there is a need to devise some appropriate indirect methods for predicting this factor in a large number of samples in water quality assessment. Forecasting DO in water can be carried out using either deterministic or statistical models. Dynamic (deterministic) models with hydrodynamic transport modeling components involve the solution of differential equations, which formulate the relevant physical, chemical, and biological mechanisms and interactions as ecological formulations (Karakaya *et al*. 2011, Chen *et al*. 2014, Rucinski *et al*. 2010). The process-based modeling approaches need approximations of several processes in most cases, and these estimations may overlook some considerable factors affecting the processes in reservoirs.

Assuming a linear relationship between the response and prediction variables in statistical models and their normal distribution can cause unreliability in nonlinear parameters. Because the DO dynamics are highly nonlinear, many useful statistical theories cannot be accurate enough for predicting this parameter. Therefore, traditional methods are no longer applicable for simulating dynamic and complicated variables. In the last two decades, several researches have been applied water quality simulation using artificial neural networks (ANN) (Keiner and Yan 1998, Zealand *et al*. 1999, Huang and Foo 2002, Misaghi *et al*. 2003, Kuo *et al*. 2004, Dogan *et al*. 2007, Musavi-Jahromi and Golabi 2008, Han *et al*. 2011, Asadollahfardi *et al*. 2011, 2013, Chen *et al*. 2014). An ANN approach has several advantages over traditional phenomenological or semi-empirical models, since they require knowing input data sets without any assumptions (Gardner and Dorling 1998, Singht *et al*. 2009). A multi-layer neural network can estimate any smooth, measurable function between input and output vectors by selecting a suitable set of connecting weights and transfer functions (Singht *et al*. 2009). An ANN consists of a system of simple interconnected processing elements. They have an ability to model any nonlinear process through a set of unidirectional weighted connections (Rene and Saidutta 2008).

2. Materials and methods

2.1 Study area

Karj Dam, also known as Amir Kabir reservoir, is located 63 kilometers northwest of Tehran and 23 kilometers north of Karaj City, Iran. The Karaj reservoir was constructed on the Karaj River, and was the first multi-purpose dam in Iran. The average annual water inflow to its reservoir is 472 million cubic meters. The bottom elevation and the normal water surface elevation of the reservoir are 1,545 meters and 1,610 meters, respectively. The Amir Kabir reservoir was built to provide potable water for Tehran and to use in agricultural development in the countryside around Karaj City. It supplies irrigation demands for over 130 million cubic meters of farmlands near Karaj. The power plant has been connected to the national electrical grid for over 52 years. The annual rainfall in the area is between 400 and 880 mm, and the mean annual temperature is between 5 and 13 degree centigrade (Ilanloo 2011). Two monitoring stations were considered for this paper, including upstream and downstream (Beylaghan) of the reservoir which are indicated in Fig. 1.

The main aim of the present work was to construct an artificial neural network (ANN) model to forecast data of dissolved oxygen (DO) water quality parameter in the Amir Kabir reservoir and

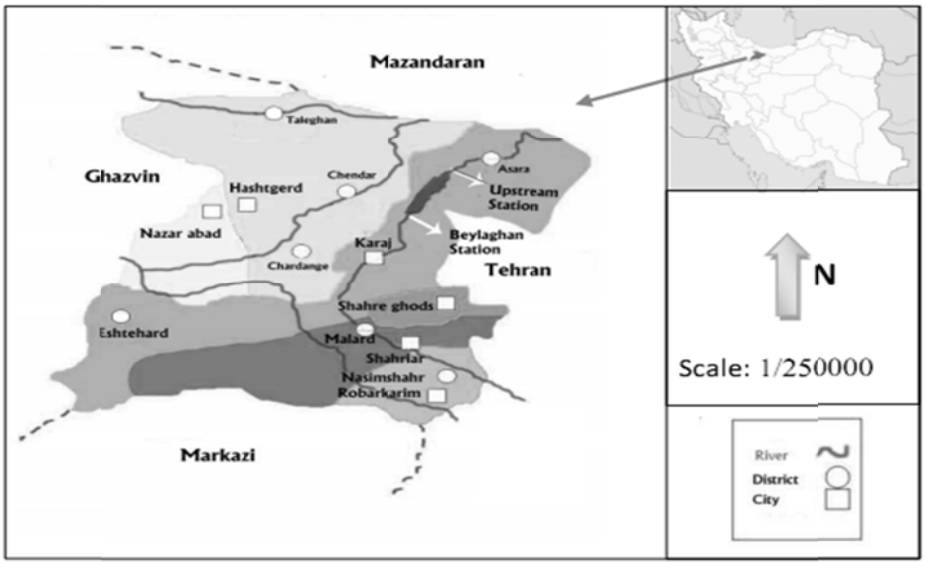

Fig. 1 The location of the study area

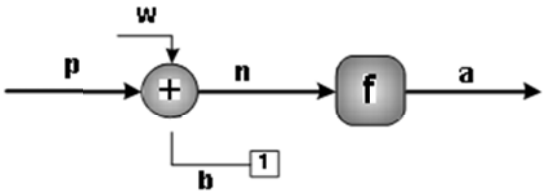

Fig. 2 Schematic of an artificial neural network (Asadollahfardi *et al*. 2013)

demonstrate its application in complex water quality data. Also we applied sensitivity analysis to recognize the most effective parameters in the prediction of the DO. Accordingly, two networks, a Multilayer Perceptron (MLP) and a Radial Basis Function (RBF) neural network were applied in two monitoring stations at the Amir Kabir reservoir in Iran.

2.2 Theory of Artificial Neural Network structure

An ANN is a data processing system, based on a model of human neurological system that consists of three unique components, including weight (w), bias (b) and a transfer function (f) (Fig. 2). Output is calculated by Eq. (1)

$$a = f(n) = f\ (wp + b) \tag{1}$$

Where "p" and "n" are the input and the output, while "a" is output and f is the transfer function. The input layer serves as an interface between the input variable data and the ANN model. Most models also contain one or two hidden layers, although more are possible. These layers perform most of the iterative calculations within the network. The output layer serves as the

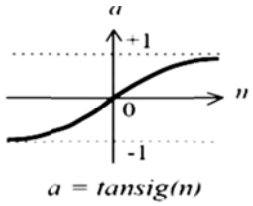

Fig. 3 Transfer function tangent sigmoid

interface between the ANN model and the end user, transforming model information into an ANN-predicted value of the output variable. The most common activation functions within the nodes is the tangent sigmoid function (Fig. 3), which produces output in the range of -1 to +1. This function introduces non-linearity into the network and provides power to capture non-linear relationships between input and output values (Baxter 2001). In this study, we used two static models, including MLP and RBF.

2.3 The MLP neural network

The MLP is a static network of the ANN (Fig. 4). The number of neurons in the hidden layers for each model can be obtained by using trial and error. The MLP with a hidden layer, tangent sigmoid transfer function and linear layer outputs can be modeled by Eqs. (2) and (3) (Menhaj 1998)

$$a_j^1(t) = F\left[\sum_{i=1}^{R} w_{i,j}^1 p_i(t) + b_j^1\right] 1 \le j \le S_1 \tag{2}$$

$$a_k^2(t) = G\left[\sum_{j=1}^{S_1} w_{k,j}^2 a_j^1(t) + b_k^2\right] 1 \le k \le S_2 \tag{3}$$

Where R is the number of input vector components; S_1 and S_2 are the number of neurons in the hidden layers and the output layers, respectively. P is the input vector. w_1, w_2 are weighting matrix in the hidden and the output layers, respectively. b_1 and b_2 are the bias vectors in the hidden layers and the output layers, respectively. G and F are the transfer functions in the hidden layers and the output layers.

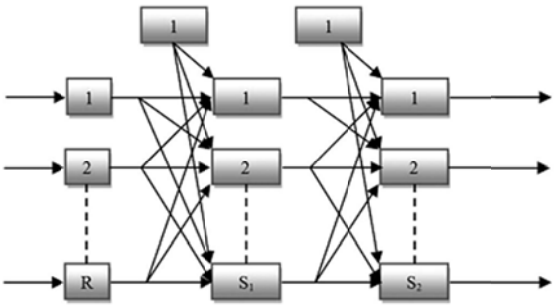

Fig. 4 The MLP with a hidden layer (Asadollahfardi *et al*. 2012)

2.4 Determination of network architecture

Selecting proper number of hidden layers in an ANN and its relationship with an optimal performance of the network is always a point of discussion. If the selected number of hidden layers is low; it is likely that mapping has not been properly estimated. On the other hand, too many hidden layers will increase network complexity. In addition, increasing the number of layers does not necessarily lead to an increase in the network accuracy. Hornik *et al*. (1989) confirmed the "universal approximator theory" which explains that a feed forward neural network with a hidden layer of a sigmoid tangent transfer function and a linear output layer would be able to estimate each complicated function (Cybenko 1989, Hornik 1991, 1993, Leshno *et al*. 1993). The rate of network efficiency depends on applying the appropriate number of neurons in the hidden layers. In this study we used an ANN with two hidden layers. The function of the hidden layers was a sigmoid tangent transfer function and the function of the output layers was considered a linear function. The number of neurons in the hidden layer is determined by trial and error method.

In learning process, a model would just repeat the labels of the samples, especially where the number of samples is small. To avoid over fitting, it is common to apply k-fold cross validation. In this method the original sample is randomly split into k almost equal sized subsamples. A model is trained using k-1 of the folds as training data; the resulting model is validated on the remaining part of the data as testing data for calculating the accuracy of the model. The cross-validation process is then repeated k times, with each of the k subsamples used exactly once as the validation data. The k results from the folds can then be averaged to make a single estimation.

2.5 Data preparation

Data collected during 2001 to 2012 was monitored by the Karaj Water Authority (Iran), and was applied for analysis. Considering the application of a sigmoid tangent transfer function in the hidden layers of the networks and the special formula of this function, the scale of input data should be changed. All used data, output and input, were transformed to -1 and +1 intervals to prevent network saturation. After finishing the process, the predicted data would be transformed back to real data. Eq. (4) is used to change the scale of the data (Razavi 2006)

$$A_s = \frac{O_t - A}{B - A} \times 2 - 1 \tag{4}$$

Where A_s and O_t are the scaled and the actual (observed) value of the DO in time t, respectively. A and B are the lowest and the highest values of a series of the DO data.

2.6 Model efficiency

To determine the amount of error in predicting the DO and the performance evaluation of the models, we used Root Mean Squared Error (RMSE) and mean bias error (MBE). The MBE provides information if the model overestimates (MBE>0) or underestimates (MBE<0) the forecasted parameter concentrations. The best score is MBE=0. They are defined as follows in Eqs. (5) and (6) (Willmott and Matsuura 2005)

$$RMSE = \sqrt{\frac{1}{n}\sum_{t=1}^{n}(O_t - F_t)^2} \tag{5}$$

$$MBE = n^{-1}\sum_{i=1}^{n} F_i - O_i \quad (6)$$

Where F_t and O_t are forecasted and observed values of DO concentration in time t respectively; and n is the number of data. Also, we used a coefficient of determination (R^2) between the observed and the predicted data to indicate the validity of the model (Eq. (7))

$$R^2 = \left\{\frac{\sum(O_i - \bar{O})(F_i - \bar{F})}{\sqrt{\sum(O_i - \bar{O})^2 - \Sigma(F_i - \bar{F})^2}}\right\}^2 \quad (7)$$

Where, O and F are observed and forecasted data, respectively. $\bar{O}$ And $\bar{F}$ are the average of O and F. Apart from the previous criteria, index of agreement (IA) was calculated to investigate how close the predicted parameters were with the observed data, Eq. (8). (Krause *et al*. 2005)

$$IA = 1 - \frac{\Sigma\overline{(F_i - O)^2}}{\overline{\overline{\Sigma|F_i - \bar{O}| + |O_i - \bar{O}||^2}}} \quad (8)$$

The index of agreement (IA) varies from 0.0 (theoretical minimum) to +1.0 (perfect agreement between the observed and predicted values).

2.7 The radial basis function (RBF) neural network

Although, the structure of the RBF is similar to the MLP, the RBF simulates an unknown water quality parameters, applying a network of Gaussian basis functions in the hidden layer (Eq. (9)) and linear activation functions in the output layer

$$f(x) = e^{-x^2/2\sigma^2} \quad (9)$$

Where x is the weighted sum of inputs to the neurons; σ is the sphere of influence or the width of the basis function, and $f(x)$ is the corresponding output of the neurons (Dawson and Wibly, 2001).

The RBF neural networks have a very simple architecture. Their structure contains an input layer, a single hidden layer, and an output layer. Training an RBF includes two steps. First, the basic functions are established using an algorithm to cluster data in the training set. Kohohen SOMs (Kohohen 1984) are a form of 'self-organizing' neural network that learn to differentiate patterns within input data. A SOM will, consequently, cluster input data according to perceived patterns without having to provide a corresponding output response. *K* means clustering, which involves the organization all objects into a predefined number of groups by minimizing the total squared Euclidean distance for each object with respect to its nearest cluster center. Other methods, such as orthogonal least squares and Maxi Min algorithms, have also been applied (Song 1996). Next, the weights linking the hidden and the output layers are calculated directly using simple matrix inversion and multiplication. The direct calculation of weights in an RBF makes it far quicker to train than an equivalent MLP (Dawson and Wibly 2001).

3. Results and discussion

Tables 1 and 2 present the statistical summary of data on the upstream and the downstream stations of Amir Kabir reservoir.

3.1 Sensitivity analysis

For selecting input parameters, we selected temperature, pH, turbidity, NO_3, Chl-a and BOD, and applied sensitivity analysis. A sensitivity analysis was performed to determine the effects of input parameters in predicting DO. We increased or decreased one of the input parameters by 20%, while the others were kept unchanged. Therefore, variations in each parameter in the prediction of DO become clear. As indicated in Fig. 5, we observed that pH and temperature effect more than 18% on prediction of the DO. It illustrates that the role of pH and temperature in DO prediction is vital. After them, BOD and Chl-a have more than 16% considerable effects on the prediction of the DO. The influence of NO_3 was less than other input parameters. The summary of the sensitivity analysis for each input parameter is summarized in the Table 3.

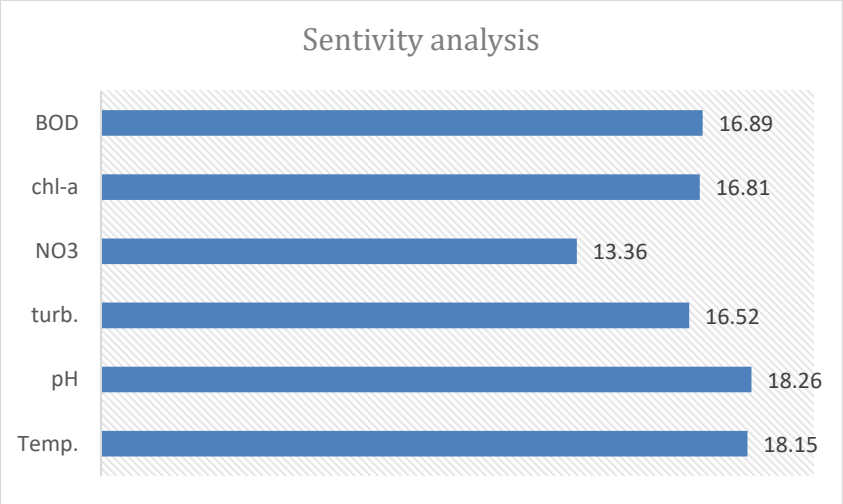

Fig. 5 the results of the sensitivity analysis

Table 1 summary of the upstream station statistical data

	BOD mg/l	DO mg/l	Temp. °C	pH	NO3 mg/l	Turbidity (NTU)	Chl-a cell/100ml
Count	120	120	120	120	120	120	120
Mean	1.63	8.64	8.50	8.23	3.48	30.28	65799
Min	0.2	6.7	1	7.62	1.7	0.7	30
10th	1	7.3	2	8	2	1.2	4416
25th	1.2	7.9	5	8.13	2	1.8	10758
75th	1.4	8.4	9	8.24	3	3	29160
120th	3.2	10.3	15	8.45	7	51.2	148480
Max	3.7	10.9	16	8.54	7.4	560	455680

Table 2 summary of the downstream (Belaghan) station statistical data

	BOD mg/l	DO mg/l	Temp. °C	pH	NO3 mg/l	Turbidity (NTU)	Chl-a cell/100ml
Count	120	120	120	120	120	120	120
Mean	1.65	8.57	10.30	8.22	3.84	11.85	68478.36
Min	0.3	6.8	2	7.87	1.7	0.5	5376
10th	1	7.5	5	8.05	2	1.5	9472
25th	1.2	7.9	8	8.14	3	2.2	20992
75th	1.5	8.4	10	8.21	3	3.5	35904
120th	3	9.9	15	8.39	7	43.2	237150
Max	3.8	10.6	20	8.42	8.1	255	404736

Table 3 the results of sensitivity analysis

Parameters	R^2 (+20%)	R^2	ΔR^2	Effect (%)
Temp.	0.6737	0.9491	0.2754	18.15
pH	0.672	0.9491	0.2771	18.26
Turb.	0.6985	0.9491	0.2506	16.52
NO_3	0.7464	0.9491	0.2027	13.36
Chl-a	0.694	0.9491	0.2551	16.81
BOD	0.6928	0.9491	0.2563	16.89

3.2 The MLP neural network results

We trained the network, using BOD, pH, temperature, turbidity, chlorophyll-a and nitrate (NO_3) as the input parameters. As illustrated in Figs. 6 and 7, the results of the MSE (training,

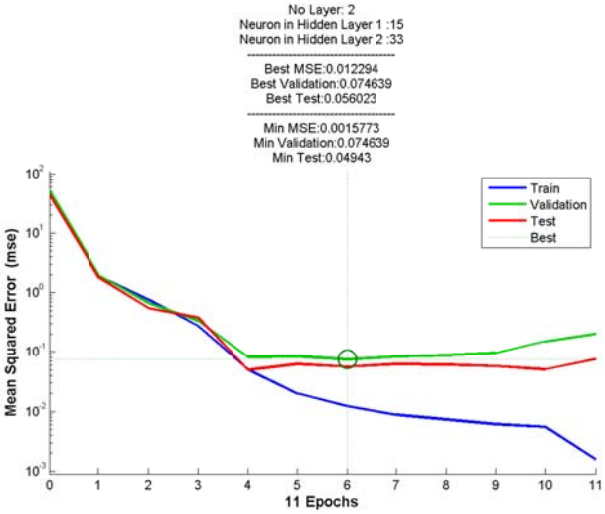

Fig. 6 training, validation and testing of errors in the MLP neural network in the upstream station

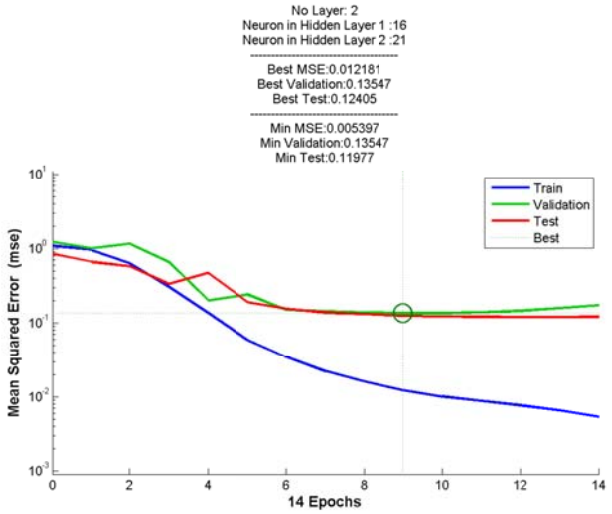

Fig. 7 training, validating and testing of errors in the MLP neural network in the downstream station

testing and validating) with different iteration numbers (Epoch) decreased as iteration increased. In MLP network, trains stopped at 11th and 14th epochs in the upstream and the downstream stations, respectively.

Tables 4 and 5 indicate the minimum amounts of error in the MLP neural networks with two hidden layers in both upstream and downstream stations. As the results indicated, the MLP models with 15 neurons in the first layer and 33 neurons in the second layer for the upstream station, and 16 neurons in the first layer and 21 neurons in the second layer for the downstream station had minimum errors. In the upstream station, the VE, MAE and RMSE were 5.5, 0.095 and 0.102, respectively. In the downstream station they were 4.35, 0.04 and 0.12, respectively. In the MLP network, the amount of Mean Bias Errors (MBE) for the upstream and the downstream stations was 0.0947 and -0.077, respectively.

Table 4 the errors in training an MLP neural network with two hidden layers in the upstream station

No. of neurons in first and second layers	VE	MAE	RMSE	No. of neurons in first and second layers	VE	MAE	RMSE
10-12	38.98	0.68	0.72	21-14	21.11	0.37	0.32
11-16	39.51	1.16	1.11	22-20	22.5	0.4	0.39
12-13	41.92	0.74	0.78	23-38	78.58	1.37	1.31
14-20	48.48	0.85	0.81	27-14	44.42	0.78	0.82
15-33	***5.5***	***0.095***	***0.12***	28-17	15.61	0.27	0.28
16-20	39.82	0.72	0.76	30-20	9.002	0.16	0.17
19-22	28.17	0.49	0.43	38-30	53.37	0.95	0.93
20-10	60.23	1.06	0.98	40-24	38.68	0.7	0.67

Table 5 the amount of errors in training an MLP neural network with two hidden layers in the downstream station

No. of neurons in first and second layers	VE	MAE	RMSE	No. of neurons in first and second layers	VE	MAE	RMSE
20-23	42.47	0.67	0.632	22-22	25.47	0.4	0.406
11-16	39.75	0.63	0.66	24-26	12.05	0.19	0.195
12-10	42.45	0.67	0.62	27-20	23.44	0.37	0.386
13-15	18.79	0.3	0.309	28-24	6.35	0.1	0.105
14-12	67.53	1.08	1.11	30-10	73.83	1.2	1.26
15-23	32.75	0.52	0.54	35-28	16.27	0.27	0.29
16-21	***4.35***	***0.04***	***0.102***	40-29	37.77	0.6	0.6525
18-15	38.9	0.607	0.616				

Figs. 8 and 9 indicate the observed and the predicted values of DO in the upstream and the downstream stations, respectively. As illustrated in these figures, the results of the observed and the predicted data have an acceptable agreement. The coefficient of determinations between the predicted and the observed data were 0.801 and 0.9039 in the upstream and the downstream stations, respectively, which means that the prediction of DO was reliable. The amount of Nash-Sutcliffe efficiency (E) and index of agreement (IA) obtained were 0.967 and 0.955, respectively, for the upstream station, and 0.983 and 0.972, respectively for the downstream station which proved the workability and efficiency of the model. As Fig. 8 presents, the values of observed DO are lower than predicted ones in the upstream station, which was proved by calculated MBE (0.0947). In the downstream station the calculated MBE was negative (-0.077), according to the Fig. 9 the predicted DO was underestimated.

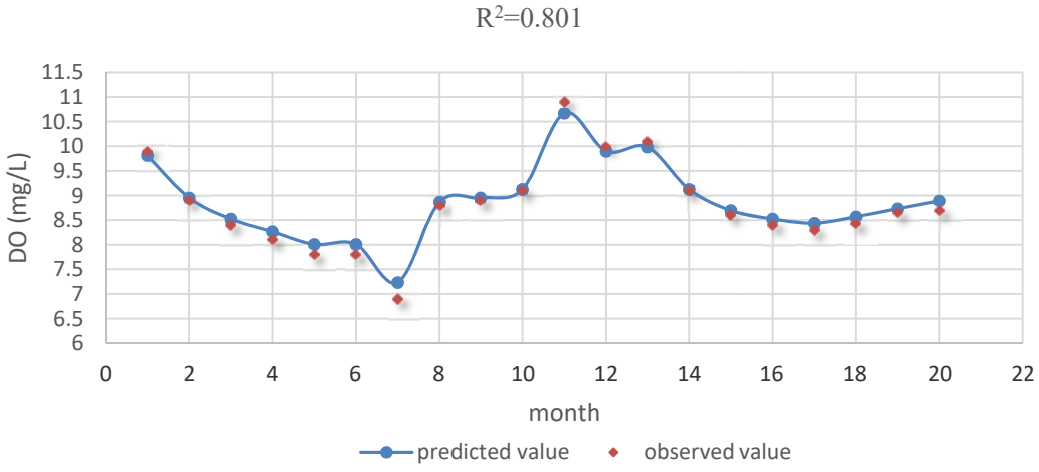

Fig. 8 comparison between the observed and the predicted DO data in the upstream station using an MLP neural network

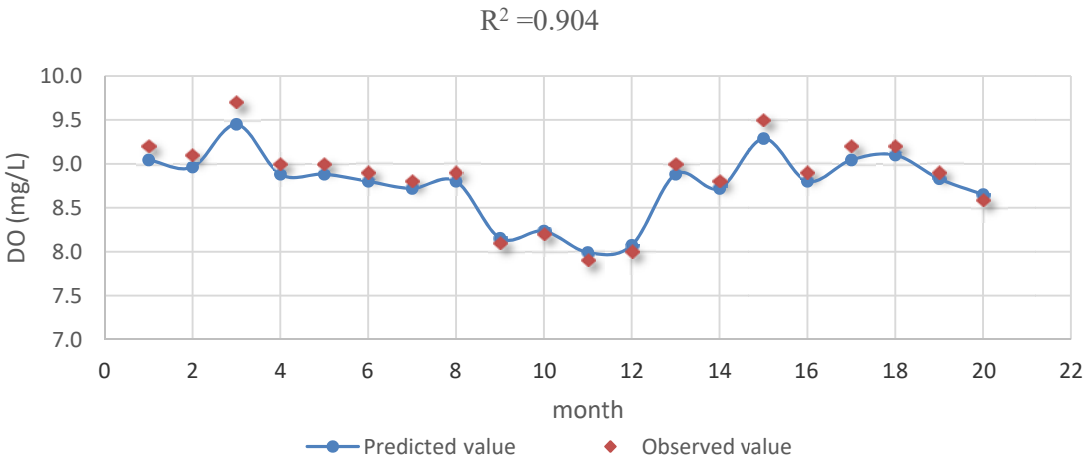

Fig. 9 comparison between the observed and the predicted DO data in the downstream station using an MLP neural network

3.3 The RBF neural network results

As mentioned previously, the RBF neural network has only one hidden layer and the minimum error was reached at 90 neurons in the hidden layer in both the upstream and the downstream stations. Figs. 10 and 11 indicate the results of training, validating and testing for the RBF neural network in both the upstream and the downstream stations with different iteration numbers (Epoch). The VE, MAE and RMSE errors for testing the RBF neural network were 3.75, 0.05 and 0.089, respectively in the upstream station. The VE, MAE and RMSE errors for testing the RBF

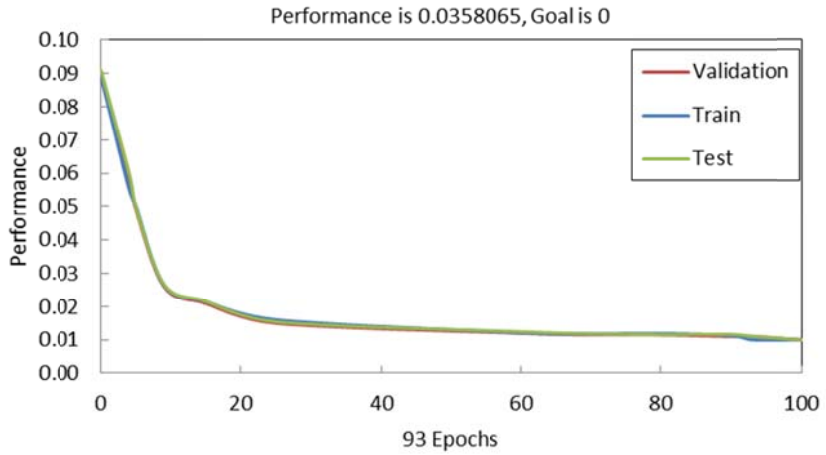

Fig. 10 training, validating and testing for the RBF neural network in the upstream station

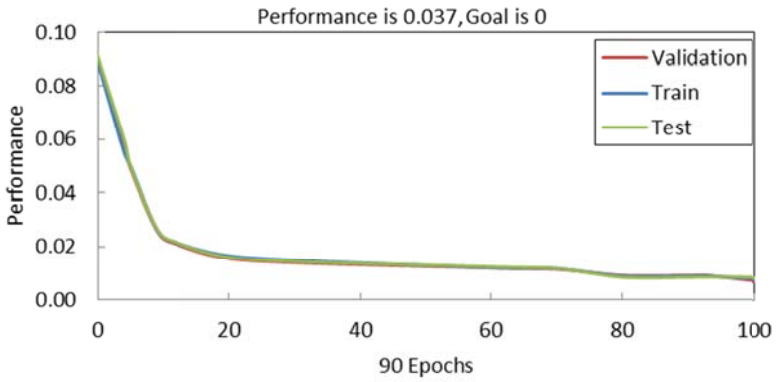

Fig. 11 training, validating and testing for the RBF neural network in the downstream station

neural network in the downstream station were 2.04, 0.027 and 0.081, respectively. The MBE in the upstream and the downstream stations were and 0.063 and 0.0126, respectively, which presents that the value of predicted DO is overestimated in both stations.

The coefficients of determination between the predicted and the observed data were 0.962 and 0.970 in the upstream and the downstream stations, respectively, which means that there is an acceptable prediction for DO in this model. The amount of Nash- Sutcliffe efficiency (E) and index of agreement (IA) obtained 0.987 and 0.991, respectively in the upstream station, and 0.995 and 0.994, respectively in the downstream station which proved the workability and efficiency of the model. Figs. 12 and 13 indicate the observed data and the predicted data on the upstream and the downstream stations, respectively. As illustrated in the figures, the results of the observed and the predicted data have a good agreement.

In this study, to avoid over fitting we used 6-fold cross validation to find the true error estimation. Therefore, we applied six sets of data, in which the testing data were changed. The results of each six subsamples validating for both MLP and RBF networks are indicated in the Table 6.

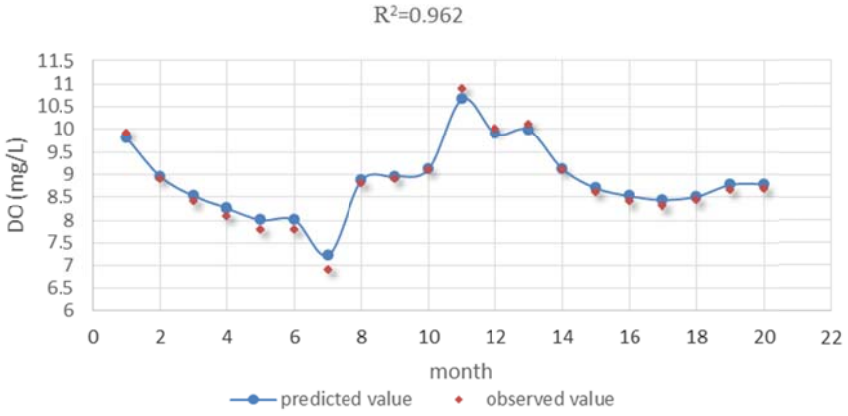

Fig. 12 comparison between the observed and the predicted DO in the upstream station using the RBF neural network

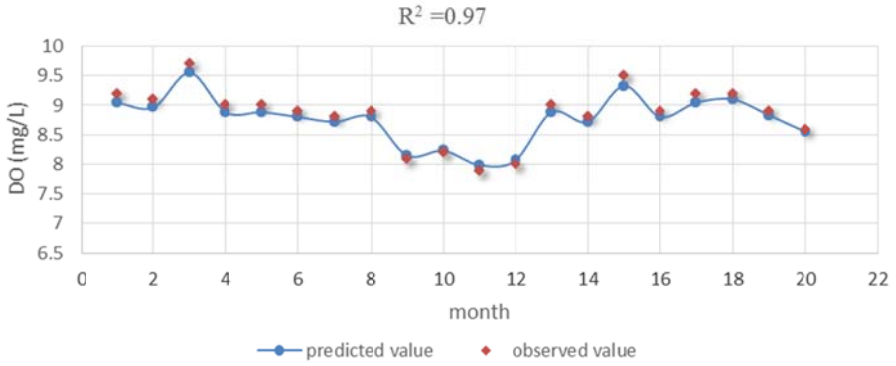

Fig. 13 comparison between the observed and the predicted DO in the downstream station using the RBF neural network

Table 6 the result of 6-fold cross validation for MLP and RBF networks

	Subsamples		NO.1	NO.2	NO.3	NO.4	NO.5	NO.6	True Error
Upstream Station	MLP	R^2	0.736	0.652	0.793	0.782	0.798	0.801	0.33167
		RMSE	0.51	0.48	0.29	0.34	0.25	0.12	
	RBF	R^2	0.939	0.945	0.953	0.951	0.955	0.962	0.1005
		RMSE	0.115	0.109	0.099	0.097	0.094	0.089	
Downstream Station	MLP	R^2	0.871	0.879	0.886	0.885	0.898	0.904	0.202
		RMSE	0.31	0.29	0.21	0.19	0.11	0.102	
	RBF	R^2	0.938	0.948	0.955	0.952	0.963	0.97	0.09867
		RMSE	0.112	0.106	0.103	0.098	0.092	0.081	

As demonstrated in the Table 6, the second set (NO.2) had the best performance. The true RMSE acquires from the average of the each subsamples error. In this study it computed, 0.332 and 0.202 for MLP networks in the upstream and downstream stations, respectively, and 0.1 and 0.099 for RBF network in the upstream and downstream stations, respectively. According to the previous results of RMSE in networks, the amount of errors in K-fold cross validation method increased.

Kuo *et al*. (2007) applied an ANN network to predict DO in the Te-Chi Reservoir, China. The coefficients of determination (R^2) for predicted and measured DO was 0.72. Ying *et al*. (2007) used the Back Propagation (BP) neural network approach to predict DO concentrations in the Yuqiao Reservoir, China. The coefficient of determination was calculated at 0.94 between the measured and simulated DO values. In our study, the coefficient of determination (R^2) obtained was 0.984 and 0.981 for DO in the upstream and downstream stations using the RBF network. In addition to R^2, the amounts of errors were less than in the mentioned studies.

4. Conclusions

The following conclusions can be summarized by considering the results of applying the multilayer perceptron (MLP) and the radial basis function (RBF) neural networks in predicting DO

in the two water quality monitoring stations at the Amir Kabir Reservoir:

• To choose the optimum variables as inputs between all the water quality parameters, a sensitivity analysis applied to demonstrate the effect of each input parameter. The results indicated that the temperature had the greatest impact, and the pH was in the second position. Biochemical Oxygen Demand (BOD) and Chlorophyll-a (Chl-a) parameters had the third and fourth roles in dissolved oxygen (DO) prediction.

• For the upstream station, the MLP with two hidden layers, which included 15 neurons in the first layer and 33 neurons in the second layer provided minimum errors. The MLP network by 16-21 neurons in first and second layer, respectively, in the downstream station had the best results.

• True RMSE in 6-fold cross validation were 0.33 and 0.100 for MLP and RBF networks, respectively in the upstream station and 0.202 and 0.098, for MLP and RBF networks, respectively in the downstream station. The MBE, using the MLP network determined that the predicted value in the upstream is overestimated, and for downstream station it is underestimated. The results of errors determined while both networks are accurate, the RBF network is more reliable.

• The coefficient of determinations in the MLP neural network were 0.801 and 0.904 for the upstream and the downstream stations, respectively. In the RBF neural network they were 0.962 and 0.97 for the upstream and the downstream stations, respectively. These results prove the better efficiency of the RBF neural network in this study.

• The amount of the Index of Agreement (IA) in both networks indicated that the RBF with an IA equal to 0.991 and 0.994 in the upstream and the downstream stations, respectively, had a better agreement compared with the MLP network, which had an IA equal to 0.955 and 0.972 for the upstream and the downstream stations, respectively.

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